EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	373	(548/316.4).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	OR	OFF	2007/06/24 13:29
L2	798	(548/311.1).CCLS.	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	OR	OFF	2007/06/24 13:30
L3	138	l1 and urea	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/06/24 13:30

EAST Search History

L4	196	l2 and urea	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/06/24 13:30
L5	6	l3 and l4	US-PGPUB; USPAT; USOCR; EPO; JPO; DERWENT; IBM_TDB	OR	ON	2007/06/24 13:30

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 NEWS PHONE    Direct Dial and Telecommunication Network Access to STN
 NEWS WWW      CAS World Wide Web Site (general information)

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FILE 'HOME' ENTERED AT 15:35:23 ON 07 AUG 2005

=> file reg
COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                         0.21       0.21

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DICTIONARY FILE UPDATES:   5 AUG 2005  HIGHEST RN 858648-31-4

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*                                                                   *
* The CA roles and document type information have been removed from *
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*                                                                   *
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for details.

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http://www.cas.org/ONLINE/DBSS/registryss.html

=>
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L1      STRUCTURE UPLOADED
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=> d
L1 HAS NO ANSWERS
L1              STR
/ Structure 1 in file .gra /


Structure attributes must be viewed using STN Express query preparation.


=> s l1
SAMPLE SEARCH INITIATED 15:36:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -  13197 TO ITERATE

 15.2% PROCESSED     2000 ITERATIONS                                50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       257059 TO   270821
PROJECTED ANSWERS:           14023 TO    17385

L2           50 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 15:36:11 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 263453 TO ITERATE

100.0% PROCESSED   263453 ITERATIONS                          14413 ANSWERS
SEARCH TIME: 00.00.03

L3        14413 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               161.33     161.54

FILE 'CAPLUS' ENTERED AT 15:36:21 ON 07 AUG 2005
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FILE COVERS 1907 - 7 Aug 2005  VOL 143 ISS 7
FILE LAST UPDATED: 5 Aug 2005  (20050805/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

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=> s l3 and ephedrine
         23578 L3
          8893 EPHEDRINE
           271 EPHEDRINES
          8933 EPHEDRINE
                 (EPHEDRINE OR EPHEDRINES)
L4           50 L3 AND EPHEDRINE

=> s l4 and urea
        201500 UREA
          9216 UREAS
        204295 UREA
                 (UREA OR UREAS)
L5           15 L4 AND UREA

=> d ibib abs hitstr tot
```

L5 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:780544 CAPLUS
DOCUMENT NUMBER: 141:301421
TITLE: Improved bioavailability and improved delivery of alkaline drugs
INVENTOR(S): Yu, Ruey J.; Van Scott, Eugene J.
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 41 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004080468	A1	20040923	WO 2004-US6699	20040305
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004214215	A1	20041028	US 2004-792273	20040304
PRIORITY APPLN. INFO.:			US 2003-452557P P	20030307
			US 2004-792273 A	20040304

OTHER SOURCE(S): MARPAT 141:301421
AB Embodiments of the invention relate to a composition, a process of making the composition, and to the use of the composition The compns. include a mol. complex formed between an alkaline pharmaceutical and at least one selected from a hydroxyacid, a polyhydroxy acid, a related acid, a lactone, or combinations thereof. The compns. provide improved bioavailability and improved delivery of the drug into the cutaneous tissues. For example, diphenhydramine hydrochloride 29 g (0.1 mol) was dissolved in water (50 mL) and 5N sodium hydroxide (20 mL) was slowly added to generate diphenhydramine as a free base as shown by the formation of oily ppts. and the change from pH 5.5 to 9.4. Gluconolactone 18 g (0.1 mol) was added to form a mol. complex between the diphenhydramine free base and gluconic acid/gluconolactone as shown by the disappearance of the oily ppts. and the change from pH 9.4 to 7.4. The solution thus obtained contained 0.1 mol diphenhydramine in mol. complex with 0.1 mol gluconic acid/gluconolactone.
This concentrated stock solution was used for various forms of topical formulations

L5 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
including oil-in-water creams, lotions, gels and solns.
IT 106516-24-9, Sertindole
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(improved bioavailability and improved delivery of alkaline drugs using hydroxy acids)
RN 106516-24-9 CAPLUS
CN 2-Imidazolidinone, 1-[2-[4-[5-chloro-1-(4-fluorophenyl)-1H-indol-3-yl]-1-piperidinyl]ethyl]- (9CI) (CA INDEX NAME)

/ Structure 2 in file .gra /

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:818401 CAPLUS
DOCUMENT NUMBER: 139:307763
TITLE: Method for the production of chiral imidazolidin-2-ones via the cyclocondensation of aminoalcohols with urea
INVENTOR(S): Ernst, Hansgeorg; Koppenhoefer, Juergen; Klein, Daniela
PATENT ASSIGNEE(S): Basf Aktiengesellschaft, Germany
SOURCE: PCT Int. Appl., 10 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003084933	A2	20031016	WO 2003-EP3615	20030408
WO 2003084933	A3	20040311		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
DE 10215845	A1	20031023	DE 2002-10215845	20020411
EP 1497267	A2	20050119	EP 2003-722413	20030408
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2005165078	A1	20050728	US 2003-510439	20030408
PRIORITY APPLN. INFO.:			DE 2002-10215845 A	20020411
			WO 2003-EP3615 W	20030408

OTHER SOURCE(S): CASREACT 139:307763; MARPAT 139:307763
GI

/ Structure 3 in file .gra /

AB Chiral imidazolidin-2-ones [I; R1 = C1-8 alkyl, cyclohexyl, (un)substituted Ph, (un)substituted naphthyl; R2 = alkyl, alkenyl, cyclohexyl, Ph, or a (un)substituted phenylalkyl; R3 = alkyl, alkenyl, cyclohexyl, (un)substituted phenyl] are prepared in high yield by reacting an aminoalc. HOCH(R1)CH(R2)NHR3 [e.g., (1S,2R)-ephedrine] or an aminoalc. salt with urea in the presence of a non-volatile ammonium salt (e.g., ammonium sulfamate), with the cyclocondensation reaction being carried out in the presence of an aprotic, polar organic solvent (e.g., NMP).
IT 92841-65-1P 112791-04-5P
RL: SPN (Synthetic preparation); PREP (Preparation)

L5 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
(method for the prodn. of chiral imidazolidin-2-ones via the cyclocondensation of aminoalcs. with urea)
RN 92841-65-1 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl-, (4R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

/ Structure 4 in file .gra /

RN 112791-04-5 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl-, (4S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 5 in file .gra /

L5 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:832746 CAPLUS
DOCUMENT NUMBER: 137:352492
TITLE: Copper-catalyzed formation of carbon-heteroatom and carbon-carbon bonds by arylation and vinylation of amines, amides, hydrazides, heterocycles, alcohols, enolates, and malonates, using aryl, heteroaryl, and vinyl halides and analogs
INVENTOR(S): Buchwald, Stephen L.; Klapars, Artis; Antilla, Jon C.; Job, Gabriel E.; Wolter, Martina; Kwong, Fuk Y.; Nordmann, Gero; Hennessy, Edward J.
PATENT ASSIGNEE(S): Massachusetts Institute of Technology, USA
SOURCE: PCT Int. Appl., 306 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002085838	A1	20021031	WO 2002-US12785	20020424
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2445159	AA	20021031	CA 2002-2445159	20020424
US 2003065187	A1	20030403	US 2002-128981	20020424
US 6759554	B2	20040706		
EP 1390340	A1	20040225	EP 2002-728925	20020424
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CN 1518534	A	20040804	CN 2002-812587	20020424
JP 2004536798	T2	20041209	JP 2002-583366	20020424
US 2004019216	A1	20040129	US 2003-435719	20030508
US 6867298	B2	20050315		

PRIORITY APPLN. INFO.: US 2001-286268P P 20010424
US 2001-348014P P 20011024
US 2001-344208P P 20011221
US 2002-128981 A3 20020424
WO 2002-US12785 W 20020424

OTHER SOURCE(S): CASREACT 137:352492; MARPAT 137:352492
GI

L5 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

/ Structure 6 in file .gra /

AB The invention relates to copper-catalyzed carbon-heteroatom and carbon-carbon bond-forming methods. More specifically, it relates to the arylation, heteroarylation, and vinylation of compds. with nucleophilic N, O, and C atoms, by aryl and vinyl halides and sulfonates, using various Cu-based catalysts and suitable ligands. The methods provide an inexpensive alternative to corresponding palladium-catalyzed reactions. Thus, the invention includes copper-catalyzed methods of forming a carbon-nitrogen bond between the nitrogen atom of an amide or amine moiety and the activated carbon of an aryl, heteroaryl, or vinyl halide or sulfonate. The invention provides similar copper-catalyzed reactions of acyl hydrazines (i.e., hydrazides). The invention further relates to copper-catalyzed arylation and vinylation of nitrogen-containing heteroaroms., e.g., indole, pyrazole, and indazole, at nitrogen. Similarly, the invention provides copper-catalyzed arylation and vinylation of alcs. at the oxygen atom. Finally, the invention provides copper-catalyzed methods of forming a carbon-carbon bond between reactants with nucleophilic carbon atoms, e.g., an enolate or malonate anion, and the activated carbon of the aryl, heteroaryl, or vinyl halides or sulfonates. Importantly, all of the invention methods are relatively inexpensive to practice due to the low cost of the copper catalysts. For example, a claimed method for amines, amides, and hydrazides involves reaction of halides and sulfonates Z-X [Z = (un)substituted aryl, heteroaryl, or alkenyl; X = iodo, Br, Cl, alkylsulfonate, arylsulfonate] with amines and derivs. R-NH-R' [R = alkyl, cycloalkyl aralkyl, aryl, heteroaryl, formyl, acyl, alkoxycarbonyl, aryloxycarbonyl, acylamino, etc.; R' = H, alkyl, cycloalkyl, (hetero)aralkyl, (hetero)aryl, formyl, acyl, amino, or amidino; with provisos] in the presence of a copper atom or ion and a ligand in the presence of a Bronsted base, yielding a corresponding arylated or vinylated product Z-NRR'. Thus, arylation of benzamide with allyl 4-iodobenzoate in dioxane solvent in the presence of CuI (catalyst), trans-1,2-cyclohexanediamine (ligand), and K3PO4 (base), at 110° in a resealable Schlenk tube, gave the expected product I in 91% yield. Similarly, 2-pyrrolidinone was N-heteroarylated by 2-iodothiophene under the same conditions to give II in quant. yield. Indole was N-arylated by 4-bromotoluene to give III in 95% yield. A similar reaction of (E)-2-undecen-1-ol with (E)-1-iodo-1-decene using CuI, 3,4,7,8-tetramethyl-1,10-phenanthroline, and Cs2CO3 in PhMe at 80°, gave 68% (E,E)-1-(dec-1-enyloxy)undec-2-ene.

IT 14599-72-5P, N-(3-Methoxyphenyl)-2-imidazolidone
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(arylation product and arylation substrate; inexpensive copper-catalyzed arylation and vinylation of amines, amides,

L5 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
heterocycles, alcs., and enolates, using aryl, heteroaryl, and vinyl halides and analogs)
RN 14599-72-5 CAPLUS
CN 2-Imidazolidinone, 1-(3-methoxyphenyl)- (9CI) (CA INDEX NAME)

/ Structure 7 in file .gra /

IT 120-93-4, 2-Imidazolidone
RL: RCT (Reactant); RACT (Reactant or reagent)
(arylation substrate; inexpensive copper-catalyzed arylation and vinylation of amines, amides, heterocycles, alcs., and enolates, using aryl, heteroaryl, and vinyl halides and analogs)
RN 120-93-4 CAPLUS
CN 2-Imidazolidinone (6CI, 8CI, 9CI) (CA INDEX NAME)

/ Structure 8 in file .gra /

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L5 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:50628 CAPLUS
DOCUMENT NUMBER: 134:117537
TITLE: Process of making imidazolidin-2-one derivatives
INVENTOR(S): Pridgen, Lendon N.
PATENT ASSIGNEE(S): SmithKline Beecham Corporation, USA; Pridgen, Karen
SOURCE: PCT Int. Appl., 12 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001004098	A1	20010118	WO 2000-US18691	20000707
W: AE, AL, AU, BA, BB, BG, BR, CA, CN, CZ, DZ, EE, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT, LV, MA, MG, MK, MN, MX, MZ, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, TZ, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1210334	A1	20020605	EP 2000-947137	20000707
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
JP 2003504357	T2	20030204	JP 2001-509709	20000707

PRIORITY APPLN. INFO.: US 1999-143110P P 19990709
WO 2000-US18691 W 20000707

OTHER SOURCE(S): MARPAT 134:117537
GI

/ Structure 9 in file .gra /

AB Imidazolidin-2-one derivs., chiral auxiliary intermediates useful in the asym. syntheses of organic compds., are prepared by the reaction of ephedrine derivs. with urea in the presence of H2NSO3NH4. Thus, heating urea 16.4, H2NSO3NH4 10.35 and L-ephedrine 14.36 kg in 36 L PhMe under N, removing PhMe at 98° and heating the residue for 1.5 h at 175-180° with removal of NH3 gave 10.7 kg crude (4R,5S)-1,5-dimethyl-4-phenylimidazolidin-2-one (I) m. 174-5° (from MeCN/H2O 93:7), [α]25D -96.3° (c 1.0, CH2Cl2); [α]25D -46° (c 1.0, MeOH).

IT 112791-04-5
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(process of making imidazolidin-2-one enantiomer from D-ephedrine and urea and ammonium sulfamate)
RN 112791-04-5 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl-, (4S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 10 in file .gra /

L5 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
IT 92841-65-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(process of making imidazolidin-2-one enantiomer from L-ephedrine and urea and ammonium sulfamate)
RN 92841-65-1 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl-, (4R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

/ Structure 11 in file .gra /

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L5 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
component from the matrix may be delayed or controlled over time so that the active component is delivered when and where it is needed to perform its intended function. Controlled release, discrete, solid particles which contain an encapsulated and/or embedded component such as a heat sensitive or readily oxidizable pharmaceutically, biol., or nutritionally active component are continuously produced without substantial destruction
of the matrix material or encapsulant.
IT 58-85-5
RL: FFD (Food or feed use); BIOL (Biological study); USES (Uses)
(encapsulation of sensitive liquid components into matrix to obtain discrete shelf-stable particles)
RN 58-85-5 CAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanoic acid, hexahydro-2-oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 12 in file .gra /

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L5 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:259972 CAPLUS
DOCUMENT NUMBER: 132:293042
TITLE: Encapsulation of sensitive liquid components into a matrix to obtain discrete shelf-stable particles
INVENTOR(S): Van Lengerich, Bernhard H.
PATENT ASSIGNEE(S): General Mills, Inc., USA
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000021504	A1	20000420	WO 1999-US20905	19991006
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2345815	AA	20000420	CA 1999-2345815	19991006
AU 9963872	A1	20000501	AU 1999-63872	19991006
AU 777977	B2	20041104		
EP 1119345	A1	20010801	EP 1999-951433	19991006
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002527375	T2	20020827	JP 2000-575480	19991006

PRIORITY APPLN. INFO.:		
US 1998-103700P	P	19981009
US 1998-109696P	P	19981124
US 1999-233443	A	19990120
WO 1999-US20905	W	19991006

AB A liquid encapsulant component which contains an active, sensitive encapsulant, such as a live microorganism or an enzyme dissolved or dispersed in a liquid plasticizer is admixed with a plasticizable matrix material. The matrix material is plasticizable by the liquid plasticizer and the encapsulation of the active encapsulant is accomplished at a low temperature and under low shear conditions. The active component is encapsulated and/or embedded in the plasticizable matrix component or material in a continuous process to produce discrete, solid particles. The liquid content of the liquid encapsulant component provides substantially
all or completely all of the liquid plasticizer needed to plasticize the matrix component to obtain a formable, extrudable, cuttable, mixture or dough. Removal of liquid plasticizer prior to extrusion is not needed to adjust the viscosity of the mixture for formability. Release of an active

L5 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:784331 CAPLUS
DOCUMENT NUMBER: 132:20747
TITLE: Surface regeneration of biosensors using a combination
of solutions based on interaction-specific optimized processes
INVENTOR(S): Andersson, Karl; Hamalainen, Markku; Malmqvist, Magnus; Roos, Hakan
PATENT ASSIGNEE(S): Biacore AB, Swed.
SOURCE: PCT Int. Appl., 133 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9963333	A1	19991209	WO 1999-SE921	19990531
W: AU, JP, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 6289286	B1	20010911	US 1998-87402	19980529
AU 9946658	A1	19991220	AU 1999-46658	19990531
AU 755181	B2	20021205		
EP 1082607	A1	20010314	EP 1999-930044	19990531
R: BE, CH, DE, FR, GB, LI, NL, SE, FI				
JP 2002517720	T2	20020618	JP 2000-552490	19990531

PRIORITY APPLN. INFO.:		
US 1998-87402	A	19980529
WO 1999-SE921	W	19990531

AB Surface regeneration of affinity biosensors and characterization of biomols. associated therewith by multivariate technique employing cocktails
of regeneration agents to optimize regeneration of biosensor surface and/or characterize biomols. associated therewith. Kits and stock solns. for
use in the context of this invention, as well as associated computer algorithms are also disclosed. Stock solns. of regeneration cocktails are
prepared and combined. Solns. are acidic, basic, ionic, organic, detergent and
chelating agent containing Biosensors for various affinity bindings are regenerated by the method; the affinity reactions are used for optimizing the regeneration process. Immuno-reactions, nucleic acid hybridization, avidin/streptavidin-biotin, hormone-hormone receptor interactions are performed with Biocore instruments and CM5 sensor chips.
IT 58-85-5
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(surface regeneration of biosensors using a combination of solns. based
on interaction-specific optimized processes)
RN 58-85-5 CAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanoic acid, hexahydro-2-oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

L5 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
/ Structure 13 in file .gra /

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L5 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:24485 CAPLUS
DOCUMENT NUMBER: 130:182498
TITLE: 1,3-Heterazolidin-2-ones as starting materials for optically active 1,3,2-oxazaborolines and 1,3,2-diazaboroline derived from ephedrines
AUTHOR(S): Cruz, Alejandro; Geniz, Erika; Contreras, Rosalinda
CORPORATE SOURCE: Departamento de Quimica, Centro de Investigacion y de Estudios Avanzados del IPN. A.P., 07000, Mex.
SOURCE: Tetrahedron: Asymmetry (1998), 9(22), 3991-3996
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:182498
GI

/ Structure 14 in file .gra /

AB Dimethylphenyloxazaboroline I derived from pseudoephedrine and trimethylphenyldiazaboroline II derived from ephedrine have been prepared from the corresponding oxazolidinone and imidazolidinone. Hydrolysis of II afforded the N,N'-dimethylphenylpropylamine III. The structures were established from 1H, 13C and 11B NMR data. The X-ray diffraction anal. of dimethylphenyldiazolidin-2-one IV was performed. Isomeric N-monoborane adducts of II were prepared, and their structures were deduced from the NMR data.

IT 112791-04-5P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and crystal structure of an optically active oxazolidinone derived from ephedrine)

RN 112791-04-5 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl-, (4S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 15 in file .gra /

REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L5 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1996:132037 CAPLUS
DOCUMENT NUMBER: 124:317052
TITLE: A New Dynamic Resolution Strategy for Asymmetric Synthesis
AUTHOR(S): Caddick, Stephen; Jenkins, Kerry
CORPORATE SOURCE: School Chemistry, Univ. Sussex, Brighton, BN1 9QJ, UK
SOURCE: Tetrahedron Letters (1996), 37(8), 1301-4
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Two different and complementary auxiliary-based dynamic resolution processes were developed; the use of crystallization-induced dynamic resolution and/or dynamic kinetic resolution enables the preparation of either enantiomeric product using a single chiral auxiliary as illustrated in the preparation of D or L-alanine derivs. The treatment of (4R-cis)-1,5-dimethyl-4-phenyl-2-imidazolidinone with 2-bromopropanoyl chloride gave a mixture of epimers, i.e., [4R-[1(2S*)4α,5α]]-2-(2-bromo-1-oxopropyl)-1,5-dimethyl-4-phenyl-2-oxazolidinone and [4R-[1(2R*)4α,5α]]-2-(2-bromo-1-oxopropyl)-1,5-dimethyl-4-phenyl-2-oxazolidinone. Treatment of this epimeric mixture with a halide source, e.g. tetrabutylammonium bromide, under equilibrating conditions allowed the isolation of [4R-[1(2R*)4α,5α]]-2-(2-bromo-1-oxopropyl)1,5-dimethyl-4-phenyl-2-oxazolidinone in 91% yield (98% enantiomeric excess). The equilibration possibly proceeds by a nucleophilic displacement process.

IT 92841-65-1P, (4R-cis)-1,5-Dimethyl-4-phenyl-2-imidazolidinone
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (bromooxopropyl)imidazolidinones via crystallization-induced dynamic kinetic resolution strategy)

RN 92841-65-1 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl-, (4R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

/ Structure 16 in file .gra /

L5 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1994:217432 CAPLUS
DOCUMENT NUMBER: 120:217432
TITLE: Ephedrine-derived imidazolidin-2-ones. Broad utility chiral auxiliaries in asymmetric synthesis
AUTHOR(S): Drewes, Siegfried E.; Malissar, Dean G. S.; Roos, Gregory H. P.
CORPORATE SOURCE: Dep. Chem., Univ. Natal, Pietermaritzburg, 3200, S. Afr.
SOURCE: Chemische Berichte (1993), 126(12), 2663-73
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 120:217432
GI

/ Structure 17 in file .gra /

AB The scope of the readily available (4R,5S)-1,5-dimethyl-4-phenylimidazolidin-2-one (I; R = Ph) and its 4-cyclohexyl analog I (R = cyclohexyl) as practical, efficient chiral auxiliaries has been demonstrated. The enolate chemical of N-acyl derivs. of I exhibits features which recommend their use in asym. synthesis. The stereoselective boron-mediated aldol as well as alkylation and acylation results are presented. The steric control benefit derived by conversion of Ph to cyclohexyl is highlighted.

IT 92841-65-1 142061-15-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation as chiral auxiliary in asym. synthesis of acyclic systems via aldol condensation, alkylation or acylation reactions)

RN 92841-65-1 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl-, (4R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

/ Structure 18 in file .gra /

RN 142061-15-2 CAPLUS
CN 2-Imidazolidinone, 4-cyclohexyl-1,5-dimethyl-, (4R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 19 in file .gra /

L5 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:174316 CAPLUS
DOCUMENT NUMBER: 116:174316
TITLE: Diastereoselective additions of alkyl-, alkenyl-, aryl- and allylcuprates to chiral unsaturated imides
AUTHOR(S): Melnyk, Oleg; Stephan, Elie; Pourcelot, Guy; Cresson, Pierre
CORPORATE SOURCE: Lab. Synth. Org., ENSCP, Paris, 75231, Fr.
SOURCE: Tetrahedron (1992), 48(5), 841-50
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 116:174316
GI

/ Structure 20 in file .gra /

AB Some diastereoselective conjugate addns. of cuprates to chiral unsatd. imides I (R = Me, Et, Pr, Ph, 4-MeC6H4) show an impressive stereoselectivity. The chiral (internal auxiliary dependent) group is easily cleaved and recycled. The steric course of these reactions seems quite general and its development synthetically promising.
IT 92841-65-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and acylation of)
RN 92841-65-1 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl-, (4R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

/ Structure 21 in file .gra /

L5 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:223259 CAPLUS
DOCUMENT NUMBER: 114:223259
TITLE: Significant differences in the structural basis of the induction of sister chromatid exchanges and chromosomal aberrations in Chinese hamster ovary cells
AUTHOR(S): Rosenkranz, Herbert S.; Ennever, Fanny K.; Dimayuga, Mario; Klopman, Gilles
CORPORATE SOURCE: Dep. Environ. Health Sci., Case West. Reserve Univ., Cleveland, OH, USA
SOURCE: Environmental and Molecular Mutagenesis (1990), 16(3), 149-77
CODEN: EMMUEG; ISSN: 0893-6692
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The structural basis of the induction of sister chromatid exchanges (SCE) and chromosomal aberrations (Cvt) in Chinese hamster ovary cells was investigated by the CASE (Computer Automated Structure Evaluation) method. Using the relevant National Toxicol. Program data bases, CASE identified a set of structural determinants responsible for the induction of SCE and another one for Cvt. A comparison between the structural determinants associated with SCE and Cvt revealed an overlap of only 22.6%, while the overlap between SCE and the determinants of mutagenicity in Salmonella is 54.5%. Apparently, the structural bases of the two phenomena differ; it is likely that SCE, but not Cvt, involves a significant electrophilic/DNA-damaging component.
IT 58-85-5, Biotin
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(genotoxicity of, computer program for evaluation of)
RN 58-85-5 CAPLUS
CN 1H-Thieno[3,4-d]imidazole-4-pentanoic acid, hexahydro-2-oxo-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 22 in file .gra /

L5 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:590602 CAPLUS
DOCUMENT NUMBER: 109:190602
TITLE: Synthesis of (R)-(+)- and (S)-(-)-α-damascone by tandem Grignard reaction-enantioselective protonation: evidence for the intermediacy of a chiral complex
AUTHOR(S): Fehr, Charles; Galindo, Jose
CORPORATE SOURCE: Res. Lab., Firmenich S. A., Geneva, CH-1211, Switz.
SOURCE: Journal of the American Chemical Society (1988), 110(20), 6909-11
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:190602
GI

/ Structure 23 in file .gra /

AB The lithium enolate of Me α-cyclogeranate (I; R, R1 = H, CO2Me) or the related ketene reacts with H2C:CHCH2MgCl to afford regio- and diastereoselectively a ketone enolate II which is then protonated with high enantioselectivity (up to 84% ee) by judicious choice of the proton source (an ephedrine derivative). A prerequisite for high enantioselectivity involves the formation of a mixed Li, Mg-complex between the enolate and a chiral alkoxide. Protonation of this complex with tert-Bu alc. is also enantioselective (62% ee). This tandem Grignard reaction-enantioselective protonation has allowed the first synthesis of enantiomerically pure (R)-(+)-(I; R = COCH:CHMe, R1 = H) and (S)-(-)-α-damascone (I; R = H, R1 = COCH:CHMe) from a common precursor.
IT 92841-65-1 112791-04-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective protonation by, of cyclohexenylbutanone enolate)
RN 92841-65-1 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl-, (4R,5S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

/ Structure 24 in file .gra /

RN 112791-04-5 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl-, (4S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

/ Structure 25 in file .gra /

IT 116559-65-0 116559-67-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(mixed-metal complexation by, prior to enantioselective protonation)
RN 116559-65-0 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl-, lithium salt, (4S-cis)- (9CI) (CA INDEX NAME)

L5 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)
Absolute stereochemistry. Rotation (+).

/ Structure 26 in file .gra /

RN 116559-67-2 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl-, lithium salt, (4R-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

/ Structure 27 in file .gra /

L5 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1976:95657 CAPLUS
DOCUMENT NUMBER: 84:95657
TITLE: Separate determination of L-ephedrine and D-ψ- ephedrine
AUTHOR(S): Mikhailova, L. N.; Preobrazhenskaya, M. N.; Kadatskii, G. M.; Sokolov, S. D.
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1975), 9(11), 49-52
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Only small amts. (.apprx.100 μg) of l- ephedrine (I) [299-42-3] and d-ψ- ephedrine (II) [90-82-4] can be separated by thin-layer chromatog. on silica in 7:3:5 CHCl3-MeOH-Me2CO. To sep. larger amts. of I and II semiquant., a mixture of them (0.2 g) is reacted with urea [57-13-6] (0.35 g) at 170-5° for 30 min and then at 200-10° for 1 hr. I is converted to (trans)-5-phenyl-3,4-dimethyl-2-imidazolidinone (III) [58337-41-0] and II to (cis)-5-phenyl-3,4-dimethyl-2-oxazolidinone (IV) [16251-46-0]. The mixture of III and IV is dissolved in 2 ml MeOH and 0.01 ml of the solution is placed on a thin layer of silica and chromatographed with Et2O, 7:5 CHCl3-Me2CO, or 5:2 Me2CO-cyclohexane. The Rf values of III are 0.35, 0.45, and 0.50, resp., and those of IV are 0.60, 0.80, and 0.95, resp.
IT 58337-41-0
RL: FORM (Formation, nonpreparative)
(formation of, from ephedrine, chromatog. determination in relation to)
RN 58337-41-0 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

/ Structure 28 in file .gra /

L5 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1957:98887 CAPLUS
DOCUMENT NUMBER: 51:98887
ORIGINAL REFERENCE NO.: 51:17805f-i,17806a
TITLE: Electronic interpretation of organic reaction mechanisms. XIX. On the reactivity and conformation of ephedrine
AUTHOR(S): Murakami, Masuo; Fukumoto, Tsugio
CORPORATE SOURCE: Osaka Univ., Sakai
SOURCE: Nippon Kagaku Zasshi (1955), 76, 270-4
CODEN: NPKZAZ; ISSN: 0369-5387
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 50, 16700h; 51, 11242d. Reaction velocity of (-)-1-chloro-2-methylamino-1-phenylpropane nitrate (I) and dl-.vphi.-1-chloro-2-methylamino-1-phenylpropane nitrate (II) with AgNO3 was investigated using NH4CNS and HNO3 titration and it was found that there was almost no difference. The reaction velocity of I with alc. KOH was studied and k2 was found to be 0.92 at -10.8° while II did not react under these conditions and at 25° k2 was less than half of that of I at -10.8°. Reaction velocity of I at 25° was too fast to measure. Treating 0.22 g. II in 20 cc. EtOH with 40 cc. 1/20N alc. KOH at 25° 3 h. gave 2,N-dimethyl-1-phenylethylenimine (III); picrate, m. 99-100°. I gave polymer on the same treatment. These facts are in line with the chlorination of n-ephedrine (IV) and .vphi.-ephedrine (V) and can be attributed to the conformation of I and II, assuming Ph and methylamino groups to be trans, Me and Cl or OH groups to be gauche in the IV system and trans in the V system. In IV systems E2 reaction took place rather than the Sn2 due to the resonance effect of the Ph group and a styrene derivative was produced, whereas in the V system, if trans elimination took place, Ph and methylamino groups would be in cis position, and thus III was produced as a result of the steric requirement. In the reaction with a ring intermediate, the V system would produce an intermediate with Ph and methylamino groups in cis position and in the V system trans. Thus, the very reactive CNBr gave stereoisomers of 3,4-dimethyl-2-imino-5-phenyloxazolidine from both IV and V systems, which was confirmed by IR analyses, while less reactive urea gave 3,4-dimethyl-5-phenylimidazolidine from IV and 3,4-dimethyl-5-phenyloxazolidine from V. Acyl migration in N-acetylephedrine (VI) and .vphi.-N-acetylephedrine (VII) was also studied and it was found that the reaction velocity of VI is about 10 times faster than that of VII. This can be explained from assumption that, due to the steric hindrance of Ph and methylamino groups in VI, the reaction proceeds via an abnormal intermediate. In fact, VI produced both IV acetate and V acetate.
IT 103774-40-9, 2-Imidazolidinone, 3,4-dimethyl-5-phenyl-
(preparation of)
RN 103774-40-9 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl- (9CI) (CA INDEX NAME)

L5 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN (Continued)

/ Structure 29 in file .gra /

L5 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1951:19034 CAPLUS
DOCUMENT NUMBER: 45:19034
ORIGINAL REFERENCE NO.: 45:3356a-e
TITLE: The conformation of the ephedrines
AUTHOR(S): Close, W. J.
CORPORATE SOURCE: Abbott Labs., N. Chicago
SOURCE: Journal of Organic Chemistry (1950), 15, 1131-4
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 45:19034
GI For diagram(s), see printed CA Issue.
AB The conformation of the ephedrine mol. is not yet settled. From the differences in reactivity of ephedrine (I) and pseudoephedrine (II) derivs., Fodor, et al. (C.A. 43, 6999d), concluded that there is some restricted rotation about the bond between the C atoms bearing the OH and the NHMe group, resp. This seems to indicate that the OH and NHMe groups are relatively distant in I and relatively close in II. Freudenberg (C.A. 26, 974; 27, 6109.9) and Welsh (C.A. 44, 5830.9) deny the existence of any restricted rotation. W. explains his results on the basis of the differences in the spatial arrangements of the groups in the diastereomers and concludes that the Ph and Me groups in I and II tend to orient themselves trans to each other. The viewpoints of Fodor and W. can be made consistent by assigning the conformations shown by III for (-)-I and IV for (+)-II, which preserves the relative configurations established for these mols. Further support for the above conformations is given by the preparation of 2-oxazolidones from I and II. Heating 40 g. dl-I.HCl and 36 g. urea 0.5 hr. at 170-5° and 1 hr. at 200-10°, treating the mixture with H2O, and washing the precipitate with 5% HCl give 48% 1,5-dimethyl-4-phenyl-2-imidazolidone, MeN.CO.NH.CHPh.CHMe (V), m. 144.5-5°. Distillation of the oily residue from the mother liquors gives a mixture, b14 202-4°, containing substantial amts. of the oxazolidone. In the same way, 20.2 g. II.HCl and urea give 73% 3,4-dimethyl-5-phenyl-2-oxazolidone, MeN.CO.O.CHPh.CHMe (VI), m. 50-1°, and dl-norephedrine-HCl and urea give 62% 4-methyl-5-phenyl-2-oxazolidone, m. 146-6.5°. The results indicate that (-)-I corresponds to V and therefore to III, and (+)-II to VI and therefore to IV.
IT 103774-40-9, 2-Imidazolidinone, 1,5-dimethyl-4-phenyl-
(preparation of)
RN 103774-40-9 CAPLUS
CN 2-Imidazolidinone, 1,5-dimethyl-4-phenyl- (9CI) (CA INDEX NAME)

/ Structure 30 in file .gra /

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